Subsurface*Topics*

INEEL Subsurface Science Initiative

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In This Issue

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SubsurfaceTopics provides technical partners and interested researchers with information and updates about the INEEL's Subsurface Science Initiative and related research.

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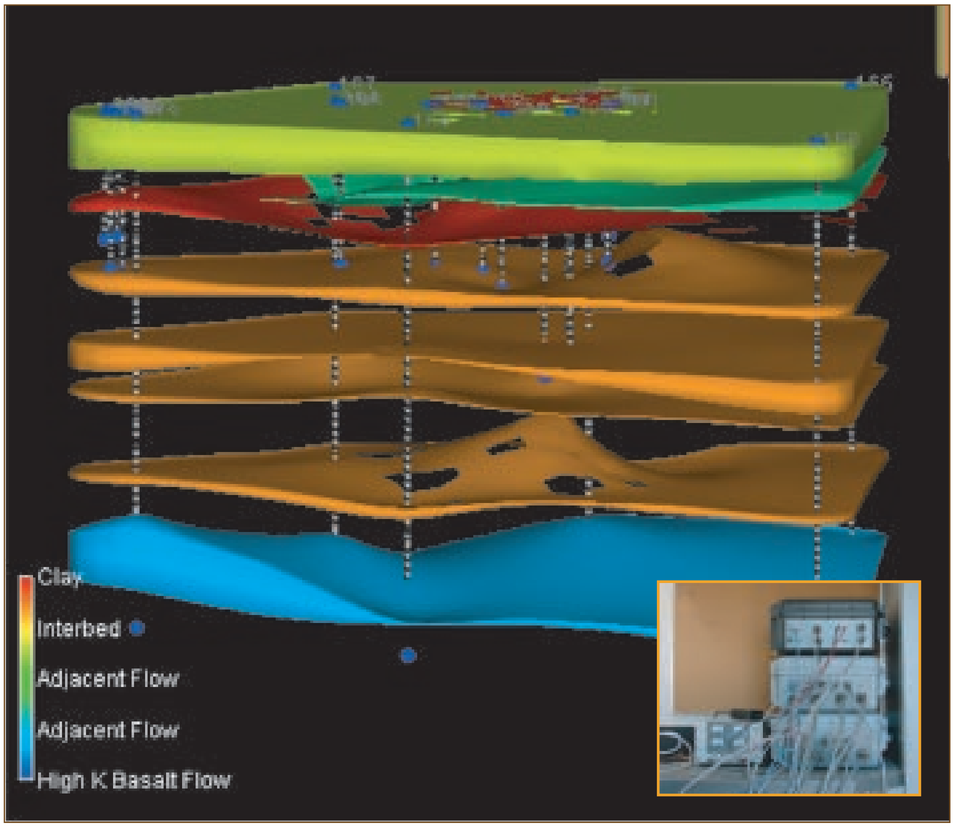

A visualization based on electrical resistivity measurements shows clay interbeds between layers of fractured basalt. The area shown is beneath the INEEL's Vadose Zone Research Park. The ability to visualize geological structure is one strength of geophysics. Today, the INEEL is directing its efforts at the next geophysical frontier—visualizing subsurface processes.

INEEL's View: The Role of Environmental Geophysics in Subsurface Science

Science is about making observations; without observations, it is difficult to test hypotheses, build models or make discoveries. In subsurface science, geophysics offers significant capabilities for observing subsurface structures and properties. However, its capabilities for observing and monitoring subsurface processes are relatively immature. This untapped potential is driving INEEL geophysics research into new areas, in particular the area of process monitoring.

Process monitoring using geophysical methods requires taking time-series measurements at spatial and temporal scales

(INEEL's view continued on page 2)

(INEEL's view continued from page 1)

relevant to the processes being studied. Time-series measurements are conceptually similar to time-lapse photography, but instead of taking a sequence of photos in which minute changes visually stand out, geophysicists take indirect measurements of resistivity, neutron absorption or other physical properties. Interpreting these measurements requires a fundamental understanding of physics to see how a process reveals itself to measurement over time.

"Quite often, colleagues in other disciplines can't make breakthroughs because they can't measure the phenomena that they *suspect* are important," said Russel Hertzog, geophysics discipline lead for the INEEL Subsurface Science Initiative. "That is where we make some of our greatest contributions."

At the INEEL, geophysicists work with biologists, physical chemists, geochemists, hydrologists and modelers to push the field of environmental geophysics into new areas. (See "Exploring Biological Reduction of Chromate," p. 3.) This multidisciplinary approach provides INEEL geophysics researchers with subsurface properties and processes in need of measurement, but they must know which properties their colleagues think are important.

"Our goal is to build strengths in areas that are important to subsurface science as a whole."

— R. Hertzog, geophysics discipline lead for the INEEL Subsurface Science Initiative

"We must be able to make a convincing case that our measurements reflect an understanding of the actual physical properties or phenomena," said Hertzog. "For that reason, we have to understand the intrinsic physics before we can develop the appropriate instruments."

"Research geophysicists must also be able to match theory with practicality," said Hertzog. In the case of sensor development, sensors must be reliable and provide good spatial and temporal resolution relevant to the particular problem. Then the data must be gathered, managed and processed into something that is meaningful to the researcher who needs it. (See "Geophysical Monitoring System Installed at EPA's Gilt Edge Superfund Site," p. 4, and "Real-Time Data Gathering," p. 7.)

While Hertzog believes geophysicists need to be versatile, he acknowledges the need for specialization and focus, too. For this reason, the SSI geophysics group includes specialists in complex resistivity, 4-D geophysics, electrode development and nuclear methods.

There are gaps that still need to be filled. According to Hertzog, uncertainty analysis in environmental geophysics is an area that has barely been addressed. To fill that void, he is actively looking for computational geophysicists or mathematical physicists who want to apply their skills to environmental problem-solving.

Another area ripe for research is interpretation of geological and physical parameters through borehole geophysics. "The oil and gas industry has developed numerous high-precision techniques that are waiting to be adapted and tailored to environmental questions," said Hertzog. "That is an area we would like to pursue."

Though the SSI group continues to build on its internal strengths by recruiting new talent, it is also solving problems through collaborations.

"It's not practical to develop in-house capabilities for everything," said Hertzog. "We are always interested in partnerships, particularly when a collaborator's strengths strongly support our program's underlying science."

Through compelling collaborations and the INEEL's own research projects, SSI researchers are helping to lift the veil on subsurface structures and processes. They are developing better methods for detecting subsurface chemical and biological processes while broadening the knowledge of geological structure and its quantification of subsurface properties.

Geophysics discipline lead, Russel Hertzog, is driving his group's research into the areas of process monitoring and environmental applications of borehole geophysics. He also hopes to expand INEEL's capabilities in uncertainty analysis to improve the field of environmental geophysics.

"Our research niches will always reflect our strengths," said Hertzog. "Our goal is to build strengths in areas that are important to subsurface science as a whole. We are the eyes and ears of the geosciences; that's our job."

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SSI Geophysics Research Focus

Ongoing SSI geophysics research projects, both internal and with collaborators, reflect the needs of the SSI and consist of:

- Time-lapse geophysical monitoring capabilities—*INEEL*
- Real-time data acquisition strategies to reduce the uncertainties in total-experiment-volume monitoring during evolving experiments—*INEEL*
- Measurement strategies to provide more detailed stratigraphic correlations for mapping subsurface structures—*INEEL*
- Geophysical instruments and methods for subsurface science—*INEEL and Center for Subsurface Sensing and Imaging Systems (CenSSIS)*
- NMR techniques to measure and understand biological processes on DNAPL transport—*INEEL and Schlumberger, Montana State University, Stanford and Sandia National Labs (reported in "New Microbe Marker Technique Benefits Environmental Research." **SubsurfaceTopics**, September 2002, p. 6., or at http://subsurface.inel.gov/information/newsletter/Vol3Iss4/marker.asp)*
- Complex resistivity to monitor biochemical changes in contaminants—*INEEL and Colorado School of Mines*
- Nuclear probes for buried TRU and MLLW measurements—*INEEL, University of Connecticut and Applied Physics Measurements, Inc. (Houston, Texas)*
- Magnetometric resistivity techniques for monitoring fluid flow—*INEEL and Multiphase Technologies (Reno, Nev.)*
- Full physics models to verify real-time EM modeling data inversions—*INEEL and University of Wisconsin–Madison*
- Fluid flow in fracture media techniques—*INEEL and University of Arizona*
- New electrodes (through metals research) for electrical resistivity tomography measurements—*INEEL and Lawrence Livermore National Laboratory*
- Polarization effects on complex resistivity electrodes and measurement systems—*INEEL and James Madison University*
- Arsenic detection and mapping in Bangladesh—*INEEL and Columbia University*
- Robotic geophysical measurements for environmental and geotechnical applications—*INEEL and Columbia University*
- Remote monitoring systems for aquifer storage and recharge in Charlotte, S.C.—*INEEL and U.S. Geological Survey*

Exploring Biological Reduction of Chromate

INEEL SSI geophysicist Birsen Canan and biologist Bill Smith are conducting experiments to detect biologically facilitated reduction of chromate. They are standing next to sand-packed columns with numerous ports for measuring the complex resistivity of solutions containing chromium.

Subsurface monitoring of contaminant biotransformation can be arduous due to the time and effort required for sampling—taking the samples, getting them to the lab and waiting for results. INEEL geophysicist Birsen Canan thinks the process could be simplified. She and a team of INEEL biologists and electrical engineers are developing a noninvasive geophysical monitoring technique for biological chromate reduction. If successful, it could lead to improved field characterization and monitoring techniques.

The team's focus is on toxic and highly soluble hexavalent chromium, originally used as a corrosion inhibitor in cooling water and discharged into the environment at the INEEL and other sites throughout the country. When hexavalent chromium is biotransformed to trivalent chromium, it is relatively insoluble and is much less harmful.

Canan and her team recently conducted an experiment in which they hoped to find a discernible signature of biological chromate reduction using nonlinear complex resistivity (NLCR). The experiment was performed using a set of sand-packed columns, each containing a different concentration of chromate. Canan measured complex resistivity over time. In several trials chromate was reduced chemically and biologically in the columns. The first run of the experiment was promising; the frequencies and

(Exploring continued on page 6)

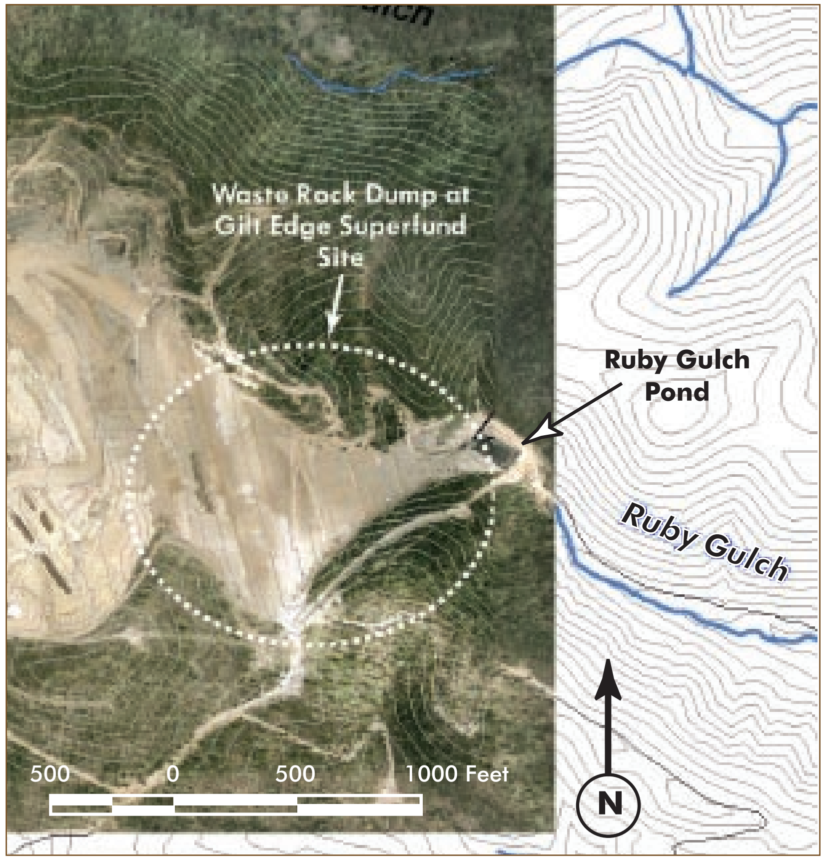
Geophysical Monitoring System Installed at EPA's Gilt Edge Superfund Site

A unique geophysical monitoring system will soon be operational at the Gilt Edge Mine Superfund site in South Dakota. The system's real-time data will help the U.S. Environmental Protection Agency (EPA) and the state of South Dakota monitor the performance of the site's huge cap. The data will also help INEEL scientists develop improved data integration and interpretation methods.

The Gilt Edge Mine is a 258-acre site on the EPA's Superfund list based on releases of cadmium, cobalt, copper, manganese, lead and zinc. The mine was developed in 1986 in South Dakota's Black Hills, but was abandoned in 1999 after its operator became insolvent.

The site consists of three open pits containing 150 million gallons of acidic, metal-laden water; a large cyanide heap leach pad; and an acid-generating rock dump. The rock dump contains approximately 20 million cubic yards of sulfidic waste rock and spent heap-leach ore material. It covers about 62 acres and is located where two headwater streams join together.

The EPA proposed a $23 million remedial action for the waste rock dump. A cap, consisting of a geotextile overlaid with soil, would be constructed to reduce acid generation by preventing water and oxygen from infiltrating through the dump. Following an August 2001 Record of Decision, the U.S. Bureau of Reclamation (BOR) completed the necessary base-



An aerial photo (top left) shows the waste rock dump at South Dakota's Gilt Edge Superfund Site with topographic contours superimposed. The photo (above), taken from the Ruby Gulch pond looking west, shows the dump prior to the installation of a protective cap. The heap leach pad is visible in the background.

grade reshaping of the dump. Before beginning cap construction, the two agencies determined that they needed to be able to monitor the remedial action's short- and long-term effectiveness. They wanted an early warning if the remedial action did not work as planned.

The EPA and BOR contacted Ken Moor, who manages INEEL's Superfund Technical Support program. Moor put them in touch with INEEL geophysicist Gail Heath. Heath suggested it was possible to build a geophysical monitoring system that could identify cap failures as well as pinpoint sources of incoming fluids. The data from this system could help scientists better understand processes beneath the liner. As a result, the agencies asked Heath and fellow INEEL geophysicist, Roelof Versteeg, to design and install a system.

"We knew we could build a monitoring system," said Heath. "The challenge was to make it provide the maximum amount of useful information in near real-time."

After carefully studying the site's characteristics and evaluating the project's goals, the team settled on a design that incorporated an electrical surface resistivity system and a suite of borehole monitoring instruments.

The surface resistivity system spans the entire cap over the waste rock dump and consists of more than 600 electrodes spaced at 25-foot intervals. The borehole monitoring instruments are placed in four pairs of wells that extend 180 feet to the bottom of the waste rock dump. One well in each pair contains electrodes and thermocouples placed at 10-foot intervals from the top to the bottom of the well. The other well contains tensiometers, suction lysimeters and gas ports at varying intervals.

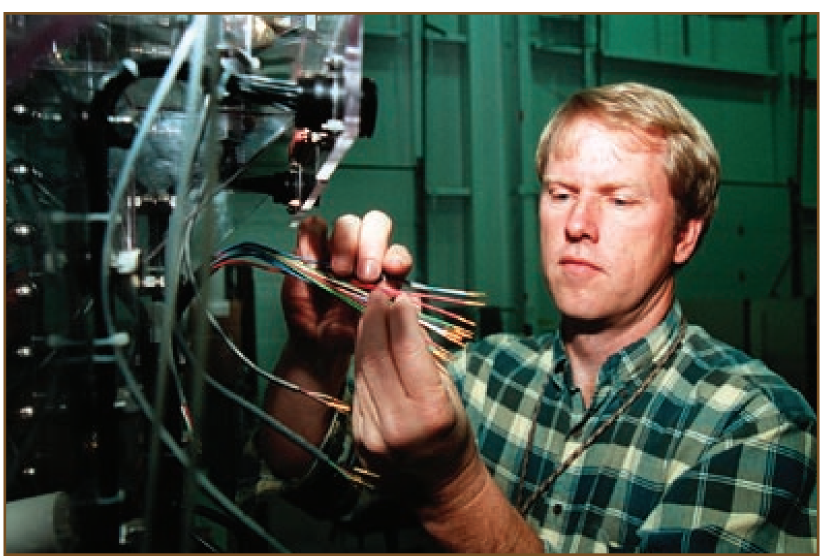
The data gathered by this system will allow scientists to map the moisture profiles and geochemical processes occurring in the material beneath the cap.

"The combination of resistivity data and direct moisture measurements will allow high confidence mapping of subsurface moisture distribution, which in turn can be used as inputs for control or mitigation of unwanted conditions," said Versteeg.

The data from the wells will also be used to validate and calibrate the surface

(Geophysical monitoring continued on page 6)

One component of the monitoring system installed at the EPA's Gilt Edge Mine site is an array of 600 stainless steel electrodes. The electrodes, connected by 18-gauge copper wires to teflon jacks with a compression fitting (top, middle), were covered with material (bottom). The electrodes for the monitoring system had to be in place before a 15-foot-thick composite cap, designed to prevent water from infiltrating into the waste rock dump, was constructed.



INEEL SSI geophysicist Gail Heath (left) helped design and install a 62-acre geophysical monitoring system for a cap at the EPA's Gilt Edge Mine Project in South Dakota.

(Exploring continued from page 3)

phase-shifts of the biologically reduced samples were distinct from the control.

Now Canan is trying to better understand the meaning of the results. "It is not enough to detect the reaction," said Canan. "I need to understand the underlying physics to develop a theoretical explanation of what it is we are measuring. Only then will I be able to develop a model to predict the reactions we are investigating."

The team will run the experiment again to improve the temporal resolution. This is needed to determine the lower threshold of chromate concentrations that can be detected using complex resistivity. This time, a biologist will take samples of the microbe population every three hours to obtain the necessary data.

The experiment's requirements have given Canan new insights into other disciplines. "The biologist will have to physically be in the lab to take samples every three hours," she said, "and the course of the experiment could take several days. I am glad I chose geophysics. My resistivity data can be collected while I sleep."

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Note: This research is funded by the INEEL's Laboratory Directed Research and Development (LDRD) program. It is being conducted by Birsen Canan, Ph.D., John Svoboda, and William A. Smith (all from the INEEL); and Gary R. Olhoeft, Ph.D. (from Colorado School of Mines).

(Geophysical monitoring continued from page 5)

resistivity system. "Resistivity provides a global view of the system conditions," said Heath, "but we need point measurements to verify any models we construct based on resistivity data."

The monitoring equipment was installed during the summer of 2002, but will not be ready for final testing until the data management components are installed in April 2003 (see "Real-Time Data Gathering," p. 7).

"With the array of instruments we have in place, we can explore any number of questions," said Heath. "These could range from how caps perform, to how they change the geochemical environment of sulfide-rich tailings over time."

The integrated use of geophysical instruments makes the monitoring system at the EPA's Gilt Edge Mine site unique. INEEL subsurface researchers have created a system that will turn raw data into information that the agencies can use to assess the cap's operational performance. At the same time, INEEL researchers will have data they can use to improve their understanding of the physical environment beneath caps.

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Note: This research is funded by the U.S. Environmental Protection Agency, Region 8, as part of the Gilt Edge Mine Project. It is being conducted by Gail Heath and Roelof Versteeg, Ph.D. (both from the INEEL).

Monitoring instruments were incorporated into the design of a geophysical monitoring system for a cap at the EPA's Gilt Edge Mine Project. The instruments were installed in four well pairs that were drilled into the rock dump (top two photos) and fitted with thermocouples, electrodes, gas ports, tensiometers and lysimeters. The data gathered by the instruments will be used to calibrate the monitoring system and aid in developing models for the dynamics of the material beneath the cap. A tube of corrugated material was installed around the top of the wells (bottom photo) to ensure accessibility after the cap was constructed.

Real-Time Data Gathering

A scientist's dream... or a potential nightmare.

A continuous stream of data will soon flow from instruments at the EPA's Gilt Edge Superfund Site. The sheer volume of information could have made it a nightmare, but INEEL SSI geophysicist Roelof Versteeg has an automated system in place to acquire, process and manage it.

"Raw resistivity data are useless to the end-user," said Versteeg. "To become meaningful information, they must be validated, inverted and visualized in a framework and manner relevant to the end-user.

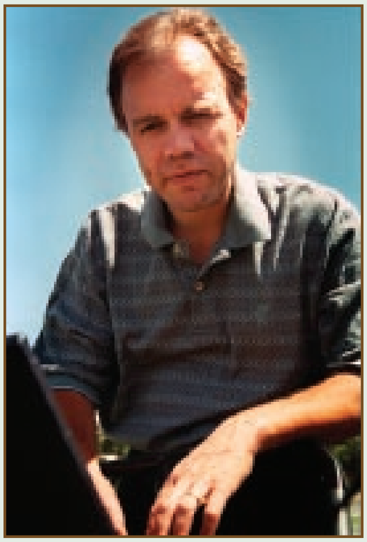
"Data management is an essential part of this process. If you don't start with a good plan, you are already sunk. Data management has to begin the moment you conceive an experiment."

Luckily, designing ways to automatically handle and process geophysical data is one of Versteeg's passions. He is particularly interested in automating and integrating raw data, then turning it into real- or near real-time information with practical value.

When Versteeg began working on the monitoring system for the Gilt Edge site, his goal was to build an automated system that answered EPA's needs. (See "Geophysical Monitoring System Installed at EPA's Gilt Edge Superfund Site," p. 4.)

The monitoring system installed for the EPA was that and more. It uses standard instrumentation that works with most commercial resistivity systems. It will not only capture and process monitoring data, it will sound a virtual alarm when cap performance parameters are out of tolerance.

The system is controlled by a dedicated computer that runs a data acquisition program and a communication program. The data acquisition program, called the resistivity commander, stores data—acquisition geometry, instrument status and time of acquisition—in flat files. The communication program, called the node commander, uses standard internet communication protocols to transfer the data through a dial-up connection to a central controller program at the INEEL.



INEEL SSI geophysicist Roelof Versteeg (above) helped design the automated geophysical monitoring system for the EPA's Gilt Edge Mine Project. Versteeg has a strong interest in automating and integrating raw data, then turning it into useful real- or near real-time information.

At the INEEL, the central controller program receives the data, hands it off to a processing program that eliminates bad data, and prepares and runs a 3-D inversion using one of a suite of inversion codes. The data are visualized and an automatic report is generated. That report is immediately accessible to the end-user through a dedicated server.

One essential part of this system is its back-end relational database where raw and processed data are stored automatically. Customized PHP (a widely-used general-purpose scripting language) scripts allow the customer to query the database, compare images and access all aspects of the data.

The system also automatically detects anomalies. "If a signature is found in the data that corresponds to moisture beneath the cap in quantities of concern, the system will notify us by both e-mail and pager," said Versteeg. "It will also provide information about the source location so we can dispatch field teams to investigate."

Versteeg believes real- or near real-time geophysical monitoring systems are the wave of the future. "The capabilities offered by data acquisition through the Internet combined with the processing power of desktop computers opens a world of practical and scientific applications," said Versteeg. "It makes the remote monitoring of a site like Gilt Edge a reasonable goal."

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Using Adaptable Data Acquisition

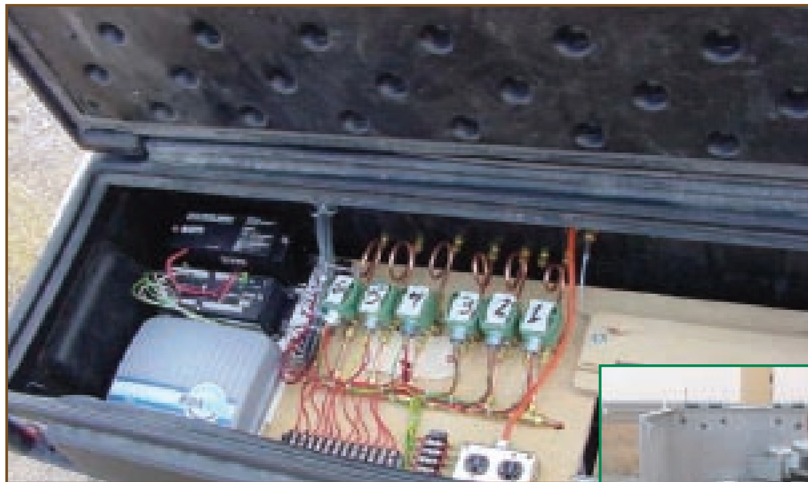
The approach that SSI geophysicist Roelof Versteeg is using to address data management and processing needs at the INEEL's Geocentrifuge Research Laboratory and at various INEEL field sites is similar to the approach he used for the EPA's Gilt Edge project in South Dakota. He is using a number of semi-autonomous data acquisition systems, typically consisting of a PC and sensors, which are capable of two-way communication for setting acquisition parameters and transmitting data.

The modularity of this approach offers several benefits, one of which is the clear separation between sensor specific software (e.g., each resistivity system has a different driver) and overall common functionality. The PHP scripts can be tailored to meet the needs of different projects. In addition, the systems can be located in a laboratory or, if necessary, halfway across the world.

Subsurface Vapor Plumes—

Changing with the Weather

The changes in barometric pressure that affect air movement above the ground's surface also affect vapor movement in the subsurface. By combining the results of field and laboratory experiments, an INEEL research team intends to create a vastly improved model for understanding subsurface vapor movement. A greater understanding of how pressure affects vapor plumes may someday enhance their monitoring and remediation.



Two vadose-zone piezometer nests (one shown at right on top of a well head) were used in INEEL research into how barometric pressure fluctuations affect subsurface vapor concentrations. Soil pressure measurements were taken every 15 minutes and concentration measurements were taken every 90 minutes from each of the six piezometer ports at a range of depths. An instrument box containing a data logger and manifold apparatus is shown above.

Throughout most of the twentieth century, diffusion was widely accepted as the dominant mechanism governing the movement of gases in the vadose zone. Diffusion models provided an adequate explanation of how vapors concentrate in the subsurface.

However, in the early 1990s, scientists at the Nevada Test Site observed that gaseous radionuclides from underground weapons tests vented to the atmosphere in months rather than in years, as predicted by diffusion theory. To explain this, they developed a theory based on the idea that barometric pumping transports gas hundreds of times faster than predicted by diffusion-based models.

Experiments by the Nevada team showed that barometric pressure fluctuations carry contaminant gases to the surface through hundreds of meters of fractured rock in a period of months, whereas contaminant gas transport by molecular diffusion alone would require decades.

Researchers at the INEEL are betting that barometric pumping also plays an important role in the movement of organic vapors.

"We suspect that atmospheric pressure changes propagated vertically in the vadose zone can be correlated with changes in the location or shape of vapor contaminant plumes," said INEEL chemical engineer Chang Oh, the principal investigator on a research project that is testing the theory.

"If so, the dynamic nature of the plume's response to atmospheric pumping may have significant implications for vapor plume modeling, besides providing strategies for monitoring and remediating these sites."

"Our goal is to collect field and laboratory data to build a computer model based on the barometric pumping theory," said team member Todd Housley. "With field and laboratory research, we may be able to explain the behavior and distribution of these organic vapor concentrations."

The team is using the vapor plume beneath the INEEL's Radioactive Waste Management Complex (RWMC) as a field site. The plume is a known source of aquifer contamination. It resulted from disposal of organic compounds, including nearly 1.8 million pounds of carbon tetrachloride, in the late 1960s.

Oh and his team designed an experiment to examine how barometric pressure fluctuations affect vapor concentrations beneath the RWMC. The team installed instruments to measure atmospheric pressures, organic vapor concentrations and soil-gas pressures in two vadose zone piezometer nests in wells 25 feet apart. Data were collected at various depths down to 150 feet below the surface. (At this location, the water table is 450 feet farther below.)

The results showed that soil pressure changes lagged behind atmospheric pressure changes and were dampened in amplitude. Chlorinated hydrocarbons and concentrations of trichloroethylene

(TCE) and carbon tetrachloride fluctuated as much as an order of magnitude over a few days. As atmospheric pressure fell, contaminant concentrations rose; as atmospheric pressure rose, contaminant concentrations fell.

The team's observations suggest that increased atmospheric pressure associated with passing high-pressure systems acts as a piston pushing the plume downward. Low atmospheric pressure appears to retard downward movement and may even tend to pull contaminants up toward the surface.

Having observed the effect of barometric pumping in the INEEL's RWMC vapor plume, the research moved to the laboratory. Team members at Brigham Young University are isolating the mechanisms of diffusive transport and pressure fluctuation in unsaturated conditions. They are measuring transport rates in conditions where variables impacting transport rates (e.g., porosity, surface adsorption, moisture content, temperature) are held constant, and the amplitude and period of atmospheric pressure fluctuations are systematically varied. Eventually, they hope to develop a quantitative understanding of the impact of pressure fluctuations.

At the INEEL, scientists have acknowledged the potential influences of barometric pumping for nearly a decade. Both research team member Jeff Sondrup and fellow scientist Swen Magnuson have included barometric pumping in subsurface transport models to predict contaminant movement in the RWMC subsurface. Until now, they lacked the data to make improvements to their models.

Now, armed with data from both the field and the laboratory, Oh's team hopes to build a model that more accurately matches the dynamics of actual plumes.

"While we recognize that barometric pumping impacts vapor transport in the vadose zone, we must improve our understanding of this phenomenon," said Sondrup. "Only then will we fully understand the risks posed by gaseous contaminants and be able to design effective remediation systems that take advantage of barometric pumping."

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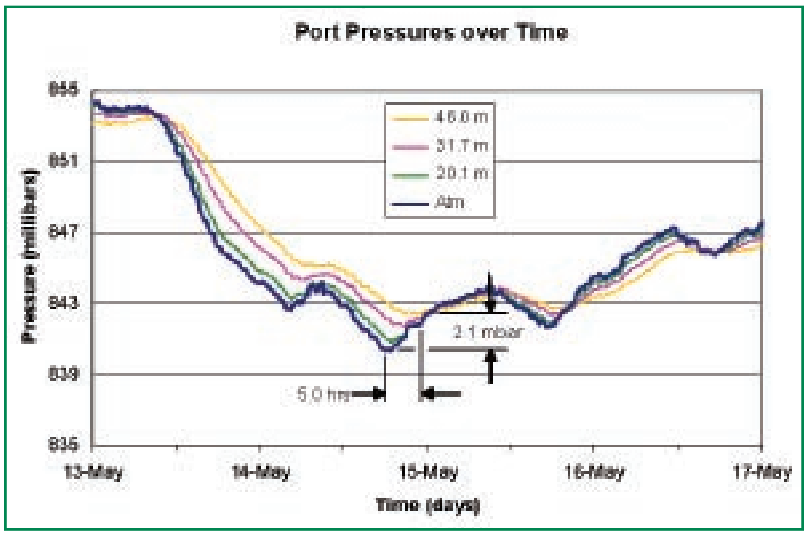
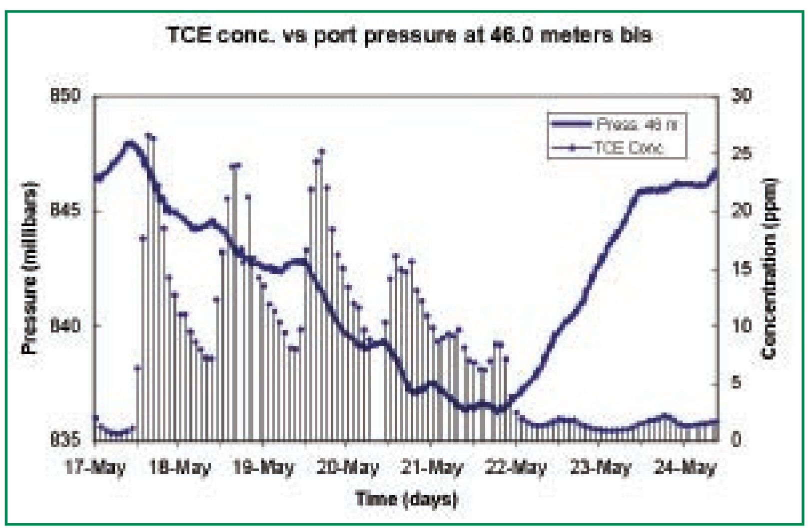
Note: This research is funded by the INEEL's Laboratory Directed Research and Development (LDRD) program. It is being conducted by Chang H. Oh, Ph.D., Todd Housley and Jeff Sondrup (all from the INEEL); and by Wayne C. Downs, Ph.D. (from Brigham Young University, Provo, Utah)





The pressure profile in the upper 46 meters of soil profile (above right) shows the lag time between changes in atmospheric pressure and changes in soil-gas pressure.

The plot of soil pressure and trichloroethylene (TCE) concentrations (below right) shows measurements at a depth of 46 meters that indicate an increase in soil pressure correlating with a decrease in TCE concentration. TCE concentrations were observed to vary more than an order of magnitude. One possible interpretation is that falling barometric pressure pulls vapor plumes up and rising barometric pressure pushes them down.

Modeling—
An Alternative to Empirical Engineering

INEEL physicist and SSI modeling lead Paul Meakin (above) is working to extend the capabilities of models for predicting subsurface contaminant behavior.

Computer models serve many functions in science. They are used to explore theories and predict the behavior of complex systems. They also help managers better understand the nature of environmental problems and how to solve them. Often, though, the underlying science is not sufficiently understood. Critical information is lacking or inappropriate computational methods are used. Then, when models are scaled up or applied to a wider range of problems, they become less accurate and often fail to predict what is observed in the field.

When models fail, there are two ways to fix them. One approach involves calibrating model parameters so that the model's code produces results that more closely match the realities of the field. The other approach involves improving the scientific basis of the model and rebuilding the code to incorporate the new science. Though it is known as an engineering laboratory, the INEEL's efforts to improve subsurface models are built on the second approach; SSI researchers use a scientific hypothesis-based method versus the empiricism of engineering.

The INEEL's SSI modeling lead, Paul Meakin, is focused on improving the value of models to subsurface research, theory and practice. He is currently working on two problems: multiphase flow in complex fracture apertures, and the behavior of colloids in fractured and porous media.

The computer modeling of multiphase flow in complex fracture apertures is challenging at any scale, so Meakin believes in beginning with small models.

"Only when you can grasp what is going on at the micro-level can you scale up your model to reflect larger and larger systems," said Meakin.

Fractures (joints and faults) are present in essentially all subsurface materials, and they may create preferred pathways for fluid transport. However, complex and dynamic fluid-fluid interfaces in fractures create difficulties for standard finite element and finite difference models. Examples include the migration of dense nonaqueous phase liquids (DNAPL) through pores or fractures and the flow of water and air in the vadose zone.

Meakin believes the best tools for modeling multiphase flow in fractures are particle-based models (including lattice-gas, lattice Boltzmann, dissipative particle dynamics, smoothed particle hydrodynamics and molecular dynamics models) and modified invasion percolation models. These approaches usually are not seen as competitive with the standard computational fluid dynamics codes, but each approach has its strengths and weaknesses.

"Particle-based simulations of multiphase flow are computationally less efficient when compared to grid-based methods," said Meakin. "But grid-based methods artificially broaden sharp interfaces, and grid entanglement becomes a serious problem for complex multi-phase flows. One example is flows in which droplets and bubbles are formed and undergo coalescence. You have to choose the computational tools that best fit the problem."

Good modeling codes also must be based on well-understood relationships. "The goal is to develop code that is based on firm theoretical foundations and is backed up by careful comparisons with experimental observations," said Meakin.

Meakin said theoreticians often prefer to compare their predictions with computer models instead of experiments, because experiments may be inadvertently influenced by processes outside the scope of the theory. However, he believes the main application of computer models is to bridge the gap between theory and experiments.

Computer models provide us with a way of synthesizing our knowledge and understanding of complex systems. A detailed comparison between computer models and experiments can reveal important gaps in our understanding or a lack of adequate information. Computer models can also be used to explore processes under extreme conditions that cannot be replicated in the laboratory or phenomena that take place on very short or very long time scales.

In theory, the iterations, comparisons and improvements in the underlying basis of models result in continuous improvements in their predictive capabilities. This appears to make models useful for policy-making. However, Meakin notes that all models have limitations that may not be appreciated.

"Models can fail for two primary reasons," said Meakin. "Either they are created with an incomplete understanding of the underlying processes, or they fail due to the input of faulty data."

Meakin recalled the modeling of ozone depletion by supersonic aircraft in the stratosphere. The project was carried out in the early 1970s as part of the U.S. Department of Transportation's Climatic Impact Assessment Program. Modelers had tens of chemical reactants and over a hundred potentially important reactions, some with difficult-to-measure rate constants.

The conclusions of the expensive multi-year program were published in six volumes of nearly 1,000 pages each in 1975. (A summary of about 250 pages and a summary of the summary were also published.) While substantial uncertainties were acknowledged, the authors of the report were confident that supersonic transports (SSTs) would deplete ozone.

Then, about a year after the report was published, Carleton J. Howard at The National Oceanic and Atmospheric Administration measured one of the difficult-to-measure rate constants again. He found that the value used in the computer models was in error by a factor of about 30. Using the new rate constant, the model showed that the Concorde SST would actually increase, rather than decrease, stratospheric ozone.

Despite their limitations, computer models are extraordinarily useful tools for improving what we know about the world. Meakin pointed to the example of modeling ozone depletion by SSTs as not a failure of the model, but an example of the problems that result if we base decisions on them without knowing the uncertainties.

"Knowing what is truly happening in a system is what research is about," said Meakin. "Otherwise, we could rely strictly on engineering empiricism and there would be little need for science. Modeling is one of the best tools we have to support the fundamental understanding of complex systems. It is one way we have to put it all together."

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Colloids and Models

The role of colloids—the tiny bits of material that can remain suspended in liquids—was once thought to be insignificant in subsurface processes. Now that scientists recognize their potential importance in contaminant transport, one of the big challenges is to develop models that accurately account for colloidal behavior in the subsurface.

One of the critical topics requiring study at the INEEL is colloid-facilitated transport of contaminants. Since the early 1990s, scientists have understood that insoluble doesn't necessarily mean immobile. Insoluble contaminants can attach themselves to colloidal particles and move freely with them. For scientists and regulators across the country, this means the role of colloids in subsurface contaminant transport can no longer be ignored.

Colloids—Finely divided dispersions of one material in a second continuous phase. The size of colloidal particles is between that of small molecules and macroscopic objects that would normally sink in the suspended phase.

Despite this, most groundwater models fail to meaningfully incorporate the role of colloid-facilitated transport. "To simply say that we need a better understanding of the role colloids play is a major understatement," says Swen Magnuson, an INEEL hydrologist who ran models for the INEEL's cleanup program.

"Without experimentally based scientific understanding of colloidal transport, we apply crude assumptions about plutonium transport that simply treat fractions of the waste as mobile. These assumptions grossly overpredict aquifer concentrations compared to current monitoring results. However, because of uncertainty associated with possible colloid-facilitated transport, plutonium is still evaluated as a special-case contaminant of concern."

Chemical precipitation is another area where colloid behavior is poorly understood. Colloids may fundamentally control or influence the kinetics of reactions, such as the formation of nanoparticles or the precipitation of solids from solutions. In groundwater, colloids act as a kind of mobile reaction surface, where chemicals can move in and out of

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solution, either precipitating on the surface of colloidal particles or sorbing onto them. Before the movement of contaminants in the subsurface can be fully modeled, it is essential that the chemistry and dynamics of these reactions be understood.

Another area of interest to INEEL researchers is the behavior of biocolloids. Since microorganisms are themselves colloidal-sized particles, colloid research has always been an area of interest for microbiologists and molecular biologists.

"It is impossible to study the movement of microbes in the subsurface without also understanding how colloids move," said INEEL microbiologist Daphne Stoner. Together with INEEL physicist Paul Meakin, Stoner is proposing to separate the biotic from abiotic factors of microbe and colloid movement in porous media so these factors can be included in fracture models.

"In one of our fracture experiments, we noticed an immediate change in flow when microbes were introduced," said Stoner. "Given the timing, we suspect that this initial effect is abiotic and related to the influence of bacteria as colloidal particles. Isolating the effect will take specifically designed experiments but will lead to better models."

INEEL microbiologist Daphne Stoner (pictured above in her laboratory) studies the interplay of fractured flow, biofilms and biocolloids.

"Understanding the behavior of colloidal particles is critically important to modeling subsurface processes," said Paul Meakin. "It is a rich area for the field of modeling and we intend to continue expanding our capabilities in this area."

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